



Ensemble Averaged Probability Density Function (APDF) for Compressible Turbulent Reacting Flows

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This report is a formal draft or working paper, intended to solicit comments and ideas from a technical peer group.

This report contains preliminary findings, subject to revision as analysis proceeds.

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Abstract

In this paper, we present a concept of the averaged probability density function (APDF) for studying compressible turbulent reacting flows. The APDF is defined as an ensemble average of the fine grained probability density function (FG-PDF) with a mass density weighting. It can be used to exactly deduce the mass density weighted, ensemble averaged turbulent mean variables. The transport equation for APDF can be derived in two ways. One is the traditional way that starts from the transport equation of FG-PDF, in which the compressible Navier-Stokes equations are embedded. The resulting transport equation of APDF is then in a traditional form that contains conditional means of all terms from the right hand side of the Navier-Stokes equations except for the chemical reaction term. These conditional means are new unknown quantities that need to be modeled. Another way of deriving the transport equation of APDF is to start directly from the ensemble averaged Navier-Stokes equations. The resulting transport equation of APDF derived from this approach appears in a closed form without any need for additional modeling. The methodology of ensemble averaging presented in this paper can be extended to other averaging procedures: for example, the Reynolds time averaging for statistically steady flow and the Reynolds spatial averaging for statistically homogeneous flow. It can also be extended to a time or spatial filtering procedure to construct the filtered density function (FDF) for the large eddy simulation (LES) of compressible turbulent reacting flows.

1.0 Introduction

The advantage of PDF method in the turbulent reacting flow simulations has been studied and examined (Refs. 1, 2, 3, and 4). Here we present the concept of an ensemble averaged probability density function (APDF) that may be considered as an extension of the conventional probability density function (PDF) method for dealing with compressible turbulent reacting flows. We do not assume that the mass density is a function of temperature and composition only, because this is only valid for the Mach number being near to zero (see Ref. 4). The APDF is defined by an ensemble average of a mass density weighted fine grained probability density function. It can be used to exactly define the mass density weighted ensemble averaged turbulent mean variables, very similar to the way in which the conventional PDF defines the turbulent mean variables.

Two ways of deriving APDF transport equation will be described in detail. One is to start from the transport equation of the fine grained probability density function (FG-PDF), in which the compressible Navier-Stokes equations are embedded. By taking ensemble average over the equation of FG-PDF, the resulting transport equation of APDF in its traditional form contains conditional means of all terms from the right hand side of the Navier-Stokes equations, except for the chemical reaction term. These conditional means are new unknown quantities that need to be modeled. Another way of deriving the transport equation of APDF is to start directly from the ensemble averaged compressible Navier-Stokes

equations. Using the relationship between APDF and the mass density weighted, ensemble averaged turbulent mean quantities, and under a “conservational” condition, the derived transport equation of APDF results in a closed form without any need for additional modeling. No terms of conditional means will appear in this conservational form of APDF equation, except when a marginal APDF equation such as the scalar APDF is considered.

The methodology of ensemble averaging procedure presented in this paper can be extended to other averaging procedures: for example, the Reynolds time average for statistically steady flows and the Reynolds spatial average for statistically homogeneous flows. In these cases, the Reynolds time (or spatial) averaged probability density function will be defined, which then defines the mass density weighted Reynolds time (or spatial) averaged turbulent mean variables.

It should be noted that for the constant density turbulent flow, the APDF will reduce exactly to the conventional PDF if the expectation of FG-PDF can be viewed as the ensemble average of FG-PDF. The conservational PDF transport equation has been reported in Reference 5.

The methodology described in this paper can also be extended to a time or spatial filtering to construct the transport equation for a mass density weighted filtered FG-PDF for large eddy simulations (LES). In this case, the mass density weighted filtered FG-PDF is named as “FMDPF” or “DW-FDF” (see Refs. 3 and 6), which is a random quantity and can be used to define the mass density weighted filtered turbulent variables to describe large scales of compressible turbulent reacting flow.

Finally, it is noted that the equations for various (PDF, APDF, DW-FDF) methods are sought to be similar, so that the solution procedures would be similar regardless of the solution variables.

2.0 Ensemble APDF

In this section, we will use the FG-PDF to define the ensemble APDF, and then explore the relationship between APDF and ensemble averaged turbulent mean variables. This will provide the basis for establishing the transport equation of APDF.

2.1 Fine Grained Probability Density Function $f'_U(V; \mathbf{x}, t)$, $f'_\Phi(\boldsymbol{\psi}; \mathbf{x}, t)$

The FG-PDF for turbulent velocity and scalars (e.g., species mass fraction or composition, internal energy) are defined as follows (Pope (Ref. 1)),

$$f'_U(V; \mathbf{x}, t) \equiv \delta(\mathbf{U}(\mathbf{x}, t) - \mathbf{V}) \equiv \prod_{i=1}^3 \delta(U_i(\mathbf{x}, t) - V_i) \quad (1)$$

$$f'_\Phi(\boldsymbol{\psi}; \mathbf{x}, t) \equiv \delta(\boldsymbol{\Phi}(\mathbf{x}, t) - \boldsymbol{\psi}) \equiv \prod_{m=1}^{M+1} \delta(\Phi_m(\mathbf{x}, t) - \psi_m) \quad (2)$$

where δ denotes the delta function, $\mathbf{U}(\mathbf{x}, t)$ is the turbulent (random) velocity vector (U_1, U_2, U_3) , $\boldsymbol{\Phi}(\mathbf{x}, t)$ is the turbulent (random) scalar array $(\Phi_1, \Phi_2, \dots, \Phi_M, \Phi_{M+1})$, for example, M species mass fractions and one internal energy $\Phi_{M+1} = e$, the $\mathbf{x}, t$ denote the physical space variable (x_1, x_2, x_3) and the time t , $\mathbf{V} \equiv (V_1, V_2, V_3)$ and $\boldsymbol{\psi} \equiv (\psi_1, \psi_2, \dots, \psi_M, \psi_{M+1})$ are the sample space variables for $\mathbf{U}(\mathbf{x}, t)$ and $\boldsymbol{\Phi}(\mathbf{x}, t)$, respectively.

2.2 Ensemble Averaged Turbulent Variables and APDF $F_U(V; \mathbf{x}, t)$, $F_\Phi(\boldsymbol{\psi}; \mathbf{x}, t)$

We start with the definition of ensemble averaged turbulent variables and the definition of ensemble averaged probability density function APDF. And then explore the relationship between the two.

2.2.1 Definition of Ensemble Averaged Turbulent Variables $\bar{\phi}(\mathbf{x}, t), \tilde{\phi}(\mathbf{x}, t)$

In the case of compressible turbulent reacting flow, we often deal with two types of ensemble averaging: one with the mass density weighting, the other without the mass density weighting. The ensemble averaged turbulent variable without the density weighting is denoted by $\bar{\phi}(\mathbf{x}, t)$ and is defined as

$$\bar{\phi}(\mathbf{x}, t) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \phi^{(n)}(\mathbf{x}, t) \quad (3)$$

where $\phi^{(n)}$ is the n -th independent realization of turbulent variables, for example, the velocity components $U_i^{(n)}$, the density $\rho^{(n)}$, pressure $P^{(n)}$, the species mass fraction $\Phi_m^{(n)}$ and the internal energy $e^{(n)} = \sum_{m=1}^M \Phi_m^{(n)} e_m^{(n)}$. N is the total number of independent realizations. The mass density weighted

ensemble averaged turbulent variable is denoted by $\tilde{\phi}(\mathbf{x}, t)$ and is defined as

$$\tilde{\phi}(\mathbf{x}, t) = \frac{\overline{\rho \phi}}{\bar{\rho}} \quad (4)$$

These ensemble averaged variables $\bar{\phi}(\mathbf{x}, t)$, $\tilde{\phi}(\mathbf{x}, t)$ represent the turbulent mean variables and are measurable in experiments. They only contain relatively low frequency and low wave number parts of the turbulent motion comparing with the non-averaged turbulent variables $\phi(\mathbf{x}, t)$.

2.2.2 Definition of Ensemble APDF

We define the following ensemble averaged probability density functions APDF:

$$\begin{aligned} F_U(V; \mathbf{x}, t) &\equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) \delta(U^{(n)}(\mathbf{x}, t) - V) \\ F_\Phi(\Psi; \mathbf{x}, t) &\equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) \delta(\Phi^{(n)}(\mathbf{x}, t) - \Psi) \end{aligned} \quad (5)$$

Obviously, thus defined $F_U(V; \mathbf{x}, t)$ or $F_\Phi(\Psi; \mathbf{x}, t)$ is no longer a random quantity. And they satisfy the following “normalization” property:

$$\begin{aligned} \int_{-\infty}^{\infty} F_U(V; \mathbf{x}, t) dV &= \int_{-\infty}^{\infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) \delta(U^{(n)}(\mathbf{x}, t) - V) dV = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) = \bar{\rho} \\ \int_{-\infty}^{\infty} F_\Phi(\Psi; \mathbf{x}, t) d\Psi &= \int_{-\infty}^{\infty} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) \delta(\Phi^{(n)}(\mathbf{x}, t) - \Psi) d\Psi = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) = \bar{\rho} \end{aligned} \quad (6)$$

Where the integration proceeds in the entire sample space of $V_i(-\infty, \infty)$ and $\Psi_i(0, 1)$.

2.2.3 Relationship Between APDF and Ensemble Averaged Turbulent Variables

With the definition of APDF described in Equation(5), we can exactly deduce the ensemble averaged turbulent variables that are defined in Equations (3) and (4). For example,

$$\begin{aligned}
\int_{-\infty}^{+\infty} V F_U(V; \mathbf{x}, t) dV &= \int_{-\infty}^{+\infty} V \left(\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) \delta(U^{(n)}(\mathbf{x}, t) - V) \right) dV \\
&= \int_{-\infty}^{+\infty} \left(\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) U^{(n)}(\mathbf{x}, t) \delta(U^{(n)}(\mathbf{x}, t) - V) \right) dV \\
&= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) U^{(n)}(\mathbf{x}, t) \\
&= \overline{\rho U} = \bar{\rho}(\mathbf{x}, t) \tilde{U}(\mathbf{x}, t)
\end{aligned} \tag{7}$$

where the sifting property of FG-PDF has been used in the second line of Equation (7).

Similarly, we have

$$\int_{-\infty}^{+\infty} \Psi F_{\Phi}(\Psi; \mathbf{x}, t) d\Psi = \overline{\rho \Phi} = \bar{\rho}(\mathbf{x}, t) \tilde{\Phi}(\mathbf{x}, t) \tag{8}$$

If we denote the left hand side of Equations (7) and (8) as a “mean” operation using APDF: $\langle U \rangle$ and $\langle \Phi \rangle$, we may write Equations (7) and (8) as

$$\langle U \rangle \equiv \int_{-\infty}^{+\infty} V F_U(V; \mathbf{x}, t) dV = \overline{\rho U} = \bar{\rho}(\mathbf{x}, t) \tilde{U}(\mathbf{x}, t) \tag{9}$$

$$\langle \Phi \rangle \equiv \int_{-\infty}^{+\infty} \Psi F_{\Phi}(\Psi; \mathbf{x}, t) d\Psi = \overline{\rho \Phi} = \bar{\rho}(\mathbf{x}, t) \tilde{\Phi}(\mathbf{x}, t) \tag{10}$$

For any function $Q(U(\mathbf{x}, t))$ or $W(\Phi(\mathbf{x}, t))$, it is easy to verify that

$$\langle Q(U) \rangle = \int_{-\infty}^{+\infty} Q(V) F_U(V; \mathbf{x}, t) dV = \bar{\rho}(\mathbf{x}, t) \tilde{Q}(U(\mathbf{x}, t)) \tag{11}$$

$$\langle W(\Phi) \rangle = \int_{-\infty}^{+\infty} W(\Psi) F_{\Phi}(\Psi; \mathbf{x}, t) d\Psi = \bar{\rho}(\mathbf{x}, t) \tilde{W}(\Phi(\mathbf{x}, t))$$

Furthermore, we may consider the derivatives ∇P , ∇U , $\nabla \Phi$ as new random quantities and legitimately write

$$\langle \nabla P \rangle = \bar{\rho} \widetilde{\nabla P}, \quad \langle \nabla U \rangle = \bar{\rho} \widetilde{\nabla U}, \quad \langle \nabla \Phi \rangle = \bar{\rho} \widetilde{\nabla \Phi} \tag{12}$$

However, because of the variable density, the mean $\langle \rangle$ does not have the differential commute property, i.e.,

$$\langle \nabla P \rangle \neq \nabla \langle P \rangle, \quad \langle \nabla U \rangle \neq \nabla \langle U \rangle, \quad \langle \nabla \Phi \rangle \neq \nabla \langle \Phi \rangle \tag{13}$$

because $\bar{\rho} \widetilde{\nabla P} \neq \nabla(\bar{\rho} \tilde{P})$, $\bar{\rho} \widetilde{\nabla U} \neq \nabla(\bar{\rho} \tilde{U})$, $\bar{\rho} \widetilde{\nabla \Phi} \neq \nabla(\bar{\rho} \tilde{\Phi})$.

It can be verified that the following “second moment” is true

$$\langle U_i U_j \rangle = \int_{-\infty}^{+\infty} V_i V_j F_U(V; \mathbf{x}, t) dV = \overline{\rho U_i U_j} = \bar{\rho}(\mathbf{x}, t) \widetilde{U_i U_j}(\mathbf{x}, t) \tag{14}$$

We can also write $\langle U_j \Phi_i \rangle$ for the joint variables as

$$\langle U_j \Phi_i \rangle = \int_{-\infty}^{+\infty} V_j \psi_i F_{U,\Phi}(V, \psi; \mathbf{x}, t) dV d\psi = \bar{\rho}(\mathbf{x}, t) \widetilde{U_j \Phi_i}(\mathbf{x}, t) \quad (15)$$

where, $F_{U,\Phi}(V, \psi; \mathbf{x}, t)$ is the velocity-scalar joint APDF defined as

$$F_{U,\Phi}(V, \psi; \mathbf{x}, t) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) \delta(U^{(n)}(\mathbf{x}, t) - V) \delta(\Phi^{(n)}(\mathbf{x}, t) - \psi) \quad (16)$$

Here, the velocity-scalar joint fine grained probability density function $f'_{U,\Phi}$ is introduced:

$$f'_{U,\Phi}(V, \psi; \mathbf{x}, t) = \delta(U(\mathbf{x}, t) - V) \delta(\Phi(\mathbf{x}, t) - \psi) \quad (17)$$

The joint APDF $F_{U,\Phi}(V, \psi; \mathbf{x}, t)$ also satisfies the normalization property:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_{U,\Phi}(V, \psi; \mathbf{x}, t) dV d\psi = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) = \bar{\rho} \quad (18)$$

2.2.4 Conditional APDF and Its Conditional Mean

From Equation(16), we may follow Pope (Ref. 1) to define a “conditional” APDF on the condition $\Phi = \psi$ as

$$F_{U|\Phi}(V|\psi; \mathbf{x}, t) \equiv \frac{F_{U,\Phi}(V, \psi; \mathbf{x}, t)}{F_{\Phi}(\psi; \mathbf{x}, t)} \quad (19)$$

and it has the following property,

$$\int_{-\infty}^{\infty} F_{U|\Phi}(V|\psi; \mathbf{x}, t) dV = 1 \quad (20)$$

The “conditional mean” will be defined as

$$\begin{aligned} \langle U(\mathbf{x}, t) | \psi \rangle &\equiv \int_{-\infty}^{+\infty} V F_{U|\Phi}(V|\psi; \mathbf{x}, t) dV = \frac{1}{F_{\Phi}(\psi; \mathbf{x}, t)} \int_{-\infty}^{+\infty} V F_{U,\Phi}(V, \psi; \mathbf{x}, t) dV \\ &= \frac{1}{F_{\Phi}} \int_{-\infty}^{+\infty} V \left(\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) \delta(U^{(n)}(\mathbf{x}, t) - V) \delta(\Phi^{(n)}(\mathbf{x}, t) - \psi) \right) dV \\ &= \frac{1}{F_{\Phi}} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) U^{(n)} \delta(\Phi^{(n)}(\mathbf{x}, t) - \psi) \end{aligned} \quad (21)$$

Then we have

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) U^{(n)} \delta(\Phi^{(n)}(\mathbf{x}, t) - \psi) = \int_{-\infty}^{+\infty} V F_{U,\Phi}(V, \psi; \mathbf{x}, t) dV = F_{\Phi} \cdot \langle U(\mathbf{x}, t) | \psi \rangle \quad (22)$$

And the total mean should be defined as

$$\begin{aligned}
& \int_{-\infty}^{+\infty} (F_{\Phi} \cdot \langle U(\mathbf{x}, t) | \Psi \rangle) d\Psi \\
&= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} V \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) \delta(U^{(n)}(\mathbf{x}, t) - V) \delta(\Phi^{(n)}(\mathbf{x}, t) - \Psi) dV d\Psi \\
&= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\mathbf{x}, t) U^{(n)}(\mathbf{x}, t) = \overline{\rho U} = \bar{\rho}(\mathbf{x}, t) \tilde{U}(\mathbf{x}, t)
\end{aligned} \tag{23}$$

Equation (22) can be extended to any other turbulent quantities, for example, $\nabla P, \nabla U, \nabla \Phi, S_i(\Phi)$:

$$\begin{aligned}
& \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\nabla P)^{(n)} \delta(U^{(n)}(\mathbf{x}, t) - V) = F_U \cdot \langle \nabla P | V \rangle \\
& \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\nabla U)^{(n)} \delta(U^{(n)}(\mathbf{x}, t) - V) = F_U \cdot \langle \nabla U | V \rangle \\
& \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)}(\nabla \Phi)^{(n)} \delta(\Phi^{(n)}(\mathbf{x}, t) - \Psi) = F_{\Phi} \cdot \langle \nabla \Phi | \Psi \rangle \\
& \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)} S_i^{(n)} \delta(\Phi^{(n)}(\mathbf{x}, t) - \Psi) = F_{\Phi} \cdot \langle S_i(\Phi) | \Psi \rangle = F_{\Phi} \cdot S_i(\Psi)
\end{aligned} \tag{24}$$

where $\nabla P, \nabla U, \nabla \Phi$ are viewed as new random variables in addition to P, U , and Φ .

3.0 Traditional Form of APDF Equations

In this section, we perform the traditional way of deriving the transport equation for APDF, i.e., we start from the equation of FG-PDF, and the resulting equation for APDF contains conditional means that require closure modeling.

3.1 Traditional Form of $F_U(V; \mathbf{x}, t)$ Equation

The transport equation for the fine grained PDF with the variable density $\rho(\mathbf{x}, t)$ can be written as (see Ref. 6):

$$\frac{\partial \rho f'_U}{\partial t} + \frac{\partial \rho U_j f'_U}{\partial x_j} = - \frac{\partial}{\partial V_i} \left\{ f'_U \left(- \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(2\mu S_{ij} - \frac{2}{3} \mu \delta_{ij} S_{kk} \right) \right) \right\} \tag{25}$$

where the compressible continuity and momentum equations (31), (32) have been applied. Applying the ensemble average operation, Equation (5), on Equation (25) and using the sifting property of FG-PDF, we may obtain

$$\begin{aligned} \frac{\partial F_U}{\partial t} + V_j \frac{\partial F_U}{\partial x_j} = & -\frac{\partial}{\partial V_i} \left\{ -\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)} \left(\frac{1}{\rho} \frac{\partial P}{\partial x_i} \right)^{(n)} (f'_U)^{(n)} \right\} \\ & -\frac{\partial}{\partial V_i} \left\{ \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \rho^{(n)} \left(\frac{1}{\rho} \frac{\partial}{\partial x_j} \left(2\mu S_{ij} - \frac{2}{3} \mu \delta_{ij} S_{kk} \right) \right)^{(n)} (f'_U)^{(n)} \right\} \end{aligned}$$

According to Equation (24), the APDF equation for the velocity can be written as

$$\frac{\partial F_U}{\partial t} + V_j \frac{\partial F_U}{\partial x_j} = -\frac{\partial}{\partial V_i} \left\{ -F_U \cdot \left\langle \frac{1}{\rho} \frac{\partial P}{\partial x_i} \middle| \mathbf{V} \right\rangle + F_U \cdot \left\langle \frac{1}{\rho} \frac{\partial}{\partial x_j} \left(2\mu S_{ij} - \frac{2}{3} \mu \delta_{ij} S_{kk} \right) \middle| \mathbf{V} \right\rangle \right\} \quad (26)$$

At this point, the velocity APDF equation is general but unclosed because of the unknown terms of the conditional means. The last term in Equation (26) is referred as the molecular mixing term in which significant modeling efforts have been devoted over several decades, nevertheless, major issues still remain. Later, we will show that when using a different way to derive the APDF equation, the molecular mixing term is in a closed form, and the pressure gradient term is also essentially closed. In addition, we noticed that the molecular mixing term is of the order of $O(1/Re)$, and may become vanishingly small when comparing with other terms in the equation in the case of large Reynolds number (Re).

3.2 Traditional Form of $F_\Phi(\boldsymbol{\psi}; \mathbf{x}, t)$ Equation

Applying the same procedure (in Section 3.1) on the following FG-PDF equation for scalars,

$$\frac{\partial \rho f'_\Phi}{\partial t} + \frac{\partial \rho U_j f'_\Phi}{\partial x_j} = -\frac{\partial}{\partial \psi_i} \left\{ f'_\Phi \left(\frac{\partial}{\partial x_j} \left(\rho \Gamma^{(i)} \frac{\partial \Phi_i}{\partial x_j} \right) + \rho S_i(\boldsymbol{\Phi}(\mathbf{x}, t)) \right) \right\} \quad (27)$$

we obtain the APDF equation for the turbulent scalars:

$$\frac{\partial F_\Phi}{\partial t} + \frac{\partial (F_\Phi \langle U_j | \boldsymbol{\psi} \rangle)}{\partial x_j} = -\frac{\partial}{\partial \psi_i} \left\{ F_\Phi \cdot \left\langle \frac{1}{\rho} \frac{\partial}{\partial x_j} \rho \Gamma^{(i)} \frac{\partial \Phi_i}{\partial x_j} \middle| \boldsymbol{\psi} \right\rangle + F_\Phi \cdot S_i(\boldsymbol{\psi}) \right\} \quad i = 1, 2, \dots, M+1 \quad (28)$$

where $S_{M+1}(\boldsymbol{\psi}) = 0$. Equation (28) is also unclosed because the conditional means are unknown. Later, we will also see that the molecular mixing term is closed when using a different way of derivation. Again, it is of the order of $O(1/Re)$ and could become vanishingly small at large Reynolds numbers.

3.3 Traditional Form of Joint APDF $F_{U,\Phi}(V, \boldsymbol{\psi}; \mathbf{x}, t)$ Equation

We may obtain the velocity-scalar joint APDF equation from the joint fine grained probability density function $f'_{U,\Phi}$ defined in Equation (17). Similar to the relationship Equation (25), we may write

$$\begin{aligned}
\frac{\partial \rho f'_{U,\Phi}}{\partial t} + \frac{\partial \rho U_j f'_{U,\Phi}}{\partial x_j} &= -\frac{\partial}{\partial V_i} \left\{ f'_{U,\Phi} \left(\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} \right) \right\} - \frac{\partial}{\partial \psi_k} \left\{ f'_{U,\Phi} \left(\frac{\partial \rho \Phi_k}{\partial t} + \frac{\partial \rho u_j \Phi_k}{\partial x_j} \right) \right\} \\
&= -\frac{\partial}{\partial V_i} \left\{ f'_{U,\Phi} \left(-\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(2\mu S_{ij} - \frac{2}{3} \mu \delta_{ij} S_{kk} \right) \right) \right\} \\
&\quad - \frac{\partial}{\partial \psi_k} \left\{ f'_{U,\Phi} \left(\frac{\partial}{\partial x_j} \left(\rho \Gamma^{(k)} \frac{\partial \Phi_k}{\partial x_j} \right) + \rho S_k(\Phi(\mathbf{x}, t)) \right) \right\}
\end{aligned} \tag{29}$$

Applying the ensemble average operation (5) on Equation (29) we obtain

$$\begin{aligned}
\frac{\partial F_{U,\Phi}}{\partial t} + V_j \frac{\partial F_{U,\Phi}}{\partial x_j} &= -\frac{\partial}{\partial V_i} \left\{ -F_{U,\Phi} \cdot \left\langle \frac{1}{\rho} \frac{\partial P}{\partial x_i} \middle| \mathbf{V}, \boldsymbol{\Psi} \right\rangle + F_{U,\Phi} \cdot \left\langle \frac{1}{\rho} \frac{\partial}{\partial x_j} \left(2\mu S_{ij} - \frac{2}{3} \mu \delta_{ij} S_{kk} \right) \middle| \mathbf{V}, \boldsymbol{\Psi} \right\rangle \right\} \\
&\quad - \frac{\partial}{\partial \psi_k} \left\{ F_{U,\Phi} \cdot \left\langle \frac{1}{\rho} \frac{\partial}{\partial x_j} \rho \Gamma^{(k)} \frac{\partial \Phi_k}{\partial x_j} \middle| \mathbf{V}, \boldsymbol{\Psi} \right\rangle + F_{U,\Phi} \cdot S_k(\boldsymbol{\Psi}) \right\}
\end{aligned} \tag{30}$$

It is easy to verify that Equation (30) will reduce to Equations (26) and (28) by an integration over the sample space $\boldsymbol{\Psi}$ and $\mathbf{V}$, respectively. The equation (30) is general and is not restricted to low Mach numbers.

4.0 Conservational Form of APDF Equations

In this section, we first review the ensemble averaged compressible Navier-Stokes equations, which are unclosed due to the unknown second order moments. Then we use the relationship between APDF and the first and second order moments described in Section 2.2 to express the ensemble averaged compressible Navier-Stokes equations in terms of an integral equation of APDF. Under a sufficient “conservation” condition, the APDF transport equations are established, which are in a closed form without additional modeling, unless a marginal APDF equation is considered.

4.1 Ensemble Averaged Compressible Navier-Stokes Equations

The Navier-Stokes equations for compressible reacting flows can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j}{\partial x_j} = 0 \tag{31}$$

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(2\rho \nu (S_{ij} - \frac{1}{3} \delta_{ij} S_{kk}) \right) \tag{32}$$

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho U_i e}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + P S_{kk} + 2\rho \nu \left(S_{ij} S_{ij} - \frac{1}{3} S_{ii} S_{kk} \right) + Q \tag{33}$$

$$\frac{\partial \rho \Phi_m}{\partial t} + \frac{\partial \rho U_i \Phi_m}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho \Gamma^{(m)} \frac{\partial \Phi_m}{\partial x_i} \right) + W_m \quad m = 1, 2, \dots, M \tag{34}$$

$$P = \rho R \sum_{m=1}^M \frac{\Phi_m T}{w_m} \quad (35)$$

$$q_i = -\rho \kappa c_v \frac{\partial T}{\partial x_i} - \sum_{m=1}^M \rho \Gamma^{(m)} h_m \frac{\partial \Phi_m}{\partial x_i} \quad (36)$$

Applying the ensemble averaging on the above equations, we obtain the following Reynolds averaged Navier-Stokes equations:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_j}{\partial x_j} = 0 \quad (37)$$

$$\frac{\partial \bar{\rho} \tilde{U}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i \tilde{U}_j}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(2\rho \nu (S_{ij} - \frac{1}{3} \delta_{ij} S_{kk}) \right) \quad (38)$$

$$\frac{\partial \bar{\rho} \tilde{e}}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i \tilde{e}}{\partial x_i} = -\frac{\partial \bar{q}_i}{\partial x_i} + \overline{P S_{kk}} + 2\rho \nu \left(S_{ij} S_{ij} - \frac{1}{3} S_{ii} S_{kk} \right) + \bar{Q} \quad (39)$$

$$\frac{\partial \bar{\rho} \tilde{\Phi}_m}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i \tilde{\Phi}_m}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho \Gamma^{(m)} \frac{\partial \Phi_m}{\partial x_i} \right) + \bar{W}_m \quad m = 1, 2, \dots, M \quad (40)$$

where

$$\bar{P} = \bar{\rho} R \sum_{m=1}^M \frac{\overline{\Phi_m T}}{w_m} = \bar{\rho} R \sum_{m=1}^M \frac{\overline{\Phi_m e}}{c_v w_m} \quad (41)$$

or

$$\bar{P} = \frac{\bar{\rho} R}{c_v} \sum_{m=1}^M \frac{\overline{\Phi_m \Phi_{M+1}}}{w_m}$$

$$\bar{q}_i = -\rho \kappa c_v \frac{\partial T}{\partial x_i} - \sum_{m=1}^M \rho \Gamma^{(m)} h_m \frac{\partial \Phi_m}{\partial x_i} \quad (42)$$

In the above equations, κ , ν and $\Gamma^{(m)}$ are the molecular heat conductivity, kinematic viscosity and the m -th species diffusivity, they have the same dimension (i.e., velocity $\cdot$ length). It is also commonly assumed that $\Gamma^{(m)}$ is the same for all species Φ_m . The h_m , T are the enthalpy of m -th species and the temperature, Q is the radiation rate, $W_m = \rho S_m$ is the chemical generation rate of m -th species, Φ_{M+1} represents the internal energy e , R is the universal gas constant. These equations are general; however, unlike the constant density flows, further approximations for the terms on their right hand side are required in order to complete the ensemble averaging process. One of such approximations leads to

$$2\rho \nu \left(S_{ij} - \frac{1}{3} \delta_{ij} S_{kk} \right) \approx \mu \left(\frac{\partial \tilde{U}_i}{\partial x_j} + \frac{\partial \tilde{U}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{U}_k}{\partial x_k} \right) \quad (43)$$

In which, we have basically neglected the variations of μ and ρ during the averaging process, the value of μ will be considered as the function of $\bar{P}, \tilde{T}, \dots$. Alternatively,

$$\overline{2\rho\nu\left(S_{ij}-\frac{1}{3}\delta_{ij}S_{kk}\right)}\approx\nu\left(\frac{\partial\bar{\rho}\tilde{U}_i}{\partial x_j}+\frac{\partial\bar{\rho}\tilde{U}_j}{\partial x_i}-\frac{2}{3}\delta_{ij}\frac{\partial\bar{\rho}\tilde{U}_k}{\partial x_k}\right) \quad (44)$$

Similarly,

$$\bar{q}_i = -\rho\kappa c_v \frac{\partial T}{\partial x_i} - \sum_{m=1}^M \overline{\rho\Gamma^{(m)}h_m \frac{\partial\Phi_m}{\partial x_i}} \approx -\kappa c_v \frac{\partial\bar{\rho}\tilde{T}}{\partial x_i} - \sum_{m=1}^M \overline{\bar{\rho}\Gamma^{(m)}h_m \frac{\partial\Phi_m}{\partial x_i}} \quad (45)$$

$$\overline{\rho\Gamma^{(m)}\frac{\partial\Phi_m}{\partial x_i}} \approx \Gamma^{(m)} \frac{\partial\bar{\rho}\tilde{\Phi}_m}{\partial x_i} \quad (46)$$

Furthermore, invoking the turbulent kinetic energy dissipation rate:

$$\overline{2\rho\nu\left(S_{ij}S_{ij}-\frac{1}{3}S_{ii}S_{kk}\right)} \equiv \bar{\rho}\tilde{\epsilon} \quad (47)$$

Where ν, κ, c_v , and $\Gamma^{(m)}$ are now considered as functions of $\bar{P}, \tilde{T}, \dots$.

Then, the ensemble averaged Navier-Stokes equations can approximately be written as

$$\frac{\partial\bar{\rho}}{\partial t} + \frac{\partial\bar{\rho}\tilde{U}_j}{\partial x_j} = 0 \quad (48)$$

$$\frac{\partial\bar{\rho}\tilde{U}_i}{\partial t} + \frac{\partial\bar{\rho}\tilde{U}_i\tilde{U}_j}{\partial x_j} = -\frac{\partial\bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\nu \left(\frac{\partial\bar{\rho}\tilde{U}_i}{\partial x_j} + \frac{\partial\bar{\rho}\tilde{U}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial\bar{\rho}\tilde{U}_k}{\partial x_k} \right) \right] \quad (49)$$

$$\frac{\partial\bar{\rho}\tilde{e}}{\partial t} + \frac{\partial\bar{\rho}\tilde{U}_i\tilde{e}}{\partial x_i} = -\frac{\partial\bar{q}_i}{\partial x_i} + \overline{PS_{kk}} + \bar{\rho}\tilde{\epsilon} + \bar{Q} \quad (50)$$

$$\frac{\partial\bar{\rho}\tilde{\Phi}_m}{\partial t} + \frac{\partial\bar{\rho}\tilde{U}_i\tilde{\Phi}_m}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial\bar{\rho}\tilde{\Phi}_m}{\partial x_i} \right) + \bar{\rho}\tilde{S}_m \quad m=1,2,\dots,M \quad (51)$$

$$\bar{P} = \bar{\rho}R \sum_{m=1}^M \frac{\overline{\Phi_m T}}{w_m} = \frac{\bar{\rho}R}{c_v} \sum_{m=1}^M \frac{\overline{\Phi_m e}}{w_m} \quad (52)$$

or

$$\bar{P} = \frac{\bar{\rho}R}{c_v} \sum_{m=1}^M \frac{\overline{\Phi_m \Phi_{M+1}}}{w_m}$$

$$\bar{q}_i = -\kappa c_v \frac{\partial\bar{\rho}\tilde{T}}{\partial x_i} - \sum_{m=1}^M \overline{\bar{\rho}\Gamma^{(m)}h_m \frac{\partial\Phi_m}{\partial x_i}} \quad (53)$$

These equations are still considered as quite general, because i) they are exact if the flow becomes incompressible, ii) all the approximations made in Equations (49), (50) and (51) are related only to the molecular diffusion terms that are less important and even become negligibly small ($1/\text{Re}$) comparing with the convection terms on the left hand side for turbulent flows at large Reynolds numbers (see Tennekes & Lumley (Ref. 7) and Pope (Ref. 1)). For the conventional unsteady Reynolds averaged Navier-Stoke simulation (URANS), Equation (48) to (51) are often used together with the further approximations for Equations (52) and (53):

$$\bar{P} = \rho R \overline{\sum_{m=1}^M \frac{\Phi_m T}{w_m}} = \overline{\left(\frac{\rho R T}{\bar{M}} \right)} \approx \frac{\bar{\rho} R \tilde{T}}{\bar{M}}, \quad \frac{1}{\bar{M}} = \sum_{m=1}^M \frac{\Phi_m}{w_m} \approx \sum_{m=1}^M \frac{\tilde{\Phi}_m}{w_m} \quad (54)$$

$$\bar{q}_i = -\kappa c_v \frac{\partial \bar{\rho} \tilde{T}}{\partial x_i} \quad (55)$$

The momentum flux $\bar{\rho} \widetilde{U_i U_j}$, the energy flux $\bar{\rho} \widetilde{U_i e}$ and the species flux $\bar{\rho} \widetilde{U_i \Phi_m}$ are considered to be critically important in URANS simulations and should be carefully modeled. Many models in the literature, from the simplest zero-equation model (Ref. 8) to the complex two-equation models (Refs. 9 and 10) have been suggested. In the following Sections 4.2 and 4.3, we will derive the APDF equations directly from Equations (48) to (53). It is important to note that in the joint PDF method, the terms corresponding to these important turbulent fluxes are always in closed forms with no need of modeling.

4.2 Conservational form of $F_U(V; x, t)$ equation

Using Equations (9) and (14), the left hand side of Equation (49) can be written as

$$\frac{\partial \bar{\rho} \tilde{U}_i}{\partial t} + \frac{\partial \bar{\rho} \widetilde{U_i U_j}}{\partial x_j} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} V_i F_U dV + \frac{\partial}{\partial x_j} \int_{-\infty}^{\infty} V_i V_j F_U dV = \int_{-\infty}^{\infty} V_i \left(\frac{\partial F_U}{\partial t} + V_j \frac{\partial F_U}{\partial x_j} \right) dV \quad (56)$$

The pressure gradient term can be written as (via Eq. (52))

$$-\frac{\partial \bar{P}}{\partial x_i} = -\frac{\partial}{\partial x_i} \left(\frac{\bar{\rho} R}{c_v} \sum_{m=1}^M \frac{\Phi_m \Phi_{M+1}}{w_m} \right) = \begin{cases} \int_{-\infty}^{\infty} V_i \frac{\partial^2}{\partial V_k \partial x_k} \left[\sum_{m=1}^M \frac{R}{c_v w_m} \left(\int_{-\infty}^{\infty} \Psi_m \Psi_{M+1} F_{U, \Phi}(\Psi, V; x, t) d\Psi \right) \right] dV \\ \text{or} \\ \int_{-\infty}^{\infty} V_i \frac{\partial^2}{\partial V_k \partial x_k} \left[\sum_{m=1}^M \frac{R}{c_v w_m} \langle \Phi_m \Phi_{M+1} | V \rangle \cdot F_U \right] dV \end{cases} \quad (57)$$

During the above arrangement, no approximations have been made other than the integration by parts and a zero integration property like Equation (59). Note that the pressure gradient term can be in a closed form only when the joint APDF, $F_{U, \Phi}$, is considered, otherwise, a conditional mean will be unavoidable. Now the molecular mixing term in Equation (49) can be written as

$$\begin{aligned}
& \frac{\partial}{\partial x_j} \mathbf{v} \left(\frac{\partial \bar{\rho} \tilde{U}_i}{\partial x_j} + \frac{\partial \bar{\rho} \tilde{U}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \bar{\rho} \tilde{U}_m}{\partial x_m} \right) \\
&= \frac{\partial}{\partial x_j} \mathbf{v} \left(\frac{\partial}{\partial x_j} \int_{-\infty}^{\infty} V_i F_U d\mathbf{V} + \frac{\partial}{\partial x_i} \int_{-\infty}^{\infty} V_j F_U d\mathbf{V} - \frac{2}{3} \delta_{ij} \frac{\partial}{\partial x_m} \int_{-\infty}^{\infty} V_m F_U d\mathbf{V} \right) \\
&= \left[\int_{-\infty}^{\infty} V_i \left(\frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_j} \right) d\mathbf{V} - \frac{\partial}{\partial x_j} \mathbf{v} \left(\frac{\partial}{\partial x_k} \int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k} (V_j F_U) d\mathbf{V} - \frac{2}{3} \delta_{kj} \frac{\partial}{\partial x_m} \int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k} (V_m F_U) d\mathbf{V} \right) \right] \\
&= \text{or} \\
& \left[-\frac{\partial}{\partial x_j} \mathbf{v} \left(\frac{\partial}{\partial x_j} \int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k} (V_k F_U) d\mathbf{V} + \frac{\partial}{\partial x_k} \int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k} (V_j F_U) d\mathbf{V} - \frac{2}{3} \delta_{kj} \frac{\partial}{\partial x_m} \int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k} (V_m F_U) d\mathbf{V} \right) \right]
\end{aligned}$$

and further rearranged as

$$\begin{aligned}
& \left[\int_{-\infty}^{\infty} V_i \left(\frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_j} \right) d\mathbf{V} - \int_{-\infty}^{\infty} V_i \frac{\partial}{\partial x_j} \left(\mathbf{v} \frac{\partial^2 V_j F_U}{\partial V_k \partial x_k} \right) d\mathbf{V} + \int_{-\infty}^{\infty} V_i \frac{2}{3} \delta_{kj} \frac{\partial}{\partial x_j} \left(\mathbf{v} \frac{\partial^2 V_m F_U}{\partial V_k \partial x_m} \right) d\mathbf{V} \right] \\
&= \text{or} \\
& \left[-\int_{-\infty}^{\infty} V_i \frac{\partial}{\partial x_j} \left(\mathbf{v} \frac{\partial^2 V_k F_U}{\partial V_k \partial x_j} \right) d\mathbf{V} - \int_{-\infty}^{\infty} V_i \frac{\partial}{\partial x_j} \left(\mathbf{v} \frac{\partial^2 V_j F_U}{\partial V_k \partial x_k} \right) d\mathbf{V} + \int_{-\infty}^{\infty} V_i \frac{2}{3} \delta_{kj} \frac{\partial}{\partial x_j} \left(\mathbf{v} \frac{\partial^2 V_m F_U}{\partial V_k \partial x_m} \right) d\mathbf{V} \right]
\end{aligned} \tag{58}$$

Note, on the third line of Equation (58), we have applied the integration by parts and the following type of zero integration similar to the one used in PDF formulations (Pope (Ref. 1)):

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial V_k} (V_i V_k F_U) d\mathbf{V} = 0 \tag{59}$$

Finally, collecting the terms that are in the integrands and factored by V_i , we obtain the following transport equation for $F_U(\mathbf{V}; \mathbf{x}, t)$ by setting the sum of the integrands to zero, which will sufficiently satisfy the Navier-Stoke equations (48), (49) and (52). We refer to this condition as the “conservation condition”.

$$\begin{aligned}
& \frac{\partial F_U}{\partial t} + V_j \frac{\partial F_U}{\partial x_j} = \frac{\partial^2}{\partial V_k \partial x_k} \left[\sum_{m=1}^M \frac{R}{c_v w_m} \langle \Phi_m \Phi_{M+1} | \mathbf{V} \rangle \cdot F_U \right] + \frac{\partial}{\partial x_j} \left(\mathbf{v} \frac{\partial F_U}{\partial x_j} \right) \\
& \quad - \frac{\partial}{\partial V_k} \left(V_j \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_k} \right) + \frac{\partial}{\partial V_k} \left(\frac{2}{3} \delta_{kj} V_m \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_m} \right) \\
& \text{or} \\
& \frac{\partial F_U}{\partial t} + V_j \frac{\partial F_U}{\partial x_j} = \frac{\partial^2}{\partial V_k \partial x_k} \left[\sum_{m=1}^M \frac{R}{c_v w_m} \langle \Phi_m \Phi_{M+1} | \mathbf{V} \rangle \cdot F_U \right] - \frac{\partial}{\partial V_k} \left(V_k \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_j} \right) \\
& \quad - \frac{\partial}{\partial V_k} \left(V_j \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_k} \right) + \frac{\partial}{\partial V_k} \left(\frac{2}{3} \delta_{kj} V_m \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_m} \right)
\end{aligned} \tag{60}$$

In Equation (60), all the terms are closed, except for the one involving the conditional mean originating from the pressure gradient. It should be noted that the unclosed term in the momentum equation, i.e., $\bar{\rho} \widetilde{U_i U_j}$, now is closed in the corresponding APDF equation while the less important molecular diffusion terms remain in closed forms.

4.3 Conservational Form of $F_\Phi(\psi; \mathbf{x}, t)$ Equation

Similarly, we may obtain the APDF equation for the scalars (i.e., species and internal energy) from Equations (50), (51) as follows: first, we write the terms on the left hand side of Equation (51) as

$$\frac{\partial \bar{\rho} \widetilde{\Phi_m}}{\partial t} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} \psi_m F_\Phi d\psi = \int_{-\infty}^{\infty} \psi_m \frac{\partial F_\Phi}{\partial t} d\psi \quad (61)$$

$$\frac{\partial \bar{\rho} \widetilde{U_i \Phi_m}}{\partial x_i} = \frac{\partial}{\partial x_i} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} V_i \psi_m F_{U,\Phi} dV d\psi = \begin{cases} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_m \left(V_i \frac{\partial}{\partial x_i} F_{U,\Phi} \right) dV d\psi \\ \text{or} \\ \int_{-\infty}^{\infty} \psi_m \left(\frac{\partial}{\partial x_i} (F_\Phi \cdot \langle U_i | \psi \rangle_L) \right) d\psi \end{cases} \quad (62)$$

Then, the terms on the right hand side of (51) can be written as

$$\frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial \bar{\rho} \widetilde{\Phi_m}}{\partial x_i} \right) = \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial}{\partial x_i} \int_{-\infty}^{\infty} \psi_m F_\Phi d\psi \right) = \begin{cases} \int_{-\infty}^{\infty} \psi_m \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial F_\Phi}{\partial x_i} \right) d\psi \\ \text{or} \\ - \int_{-\infty}^{\infty} \psi_m \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial^2 \psi_k F_\Phi}{\partial \psi_k \partial x_i} \right) d\psi \end{cases} \quad (63)$$

$$\bar{\rho} \widetilde{S_m} = \int_{-\infty}^{\infty} S_m(\psi) F_\Phi d\psi = - \int_{-\infty}^{\infty} \psi_m \frac{\partial (S_k F_\Phi)}{\partial \psi_k} d\psi \quad (64)$$

Where in Equations (63) and (64), we have applied the integration by parts and zero integrations similar to Equation (59). Collecting all the integrand terms that factored by ψ_m , and invoking the sufficient, conservation condition, we obtain

$$\begin{aligned} \frac{\partial F_\Phi}{\partial t} + \frac{\partial (F_\Phi \cdot \langle U_i | \psi \rangle)}{\partial x_i} &= \left\{ \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial F_\Phi}{\partial x_i} \right) - \frac{\partial}{\partial \psi_k} [F_\Phi \cdot S_k(\psi)] \right\}, \quad k = 1, 2, \dots, M+1 \\ \text{or} \\ \frac{\partial F_\Phi}{\partial t} + \frac{\partial (F_\Phi \cdot \langle U_i | \psi \rangle)}{\partial x_i} &= - \frac{\partial}{\partial \psi_k} \left\{ \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \psi_k \frac{\partial F_\Phi}{\partial x_i} \right) + F_\Phi \cdot S_k(\psi) \right\}, \quad k = 1, 2, \dots, M+1 \end{aligned} \quad (65)$$

This equation also represents the equation of internal energy when $S_{M+1}(\Psi) = 0$ and other source terms in Equation (50) are neglected. Equation (65) is essentially closed if we consider the joint APDF $F_{U,\Phi}$. For the marginal F_Φ , the convection term is not closed because of the conditional mean $\langle U_i | \Psi \rangle$. Then, this critically important term, corresponding to $\bar{\rho} \widetilde{U_i \Phi_m}$ in Equation (51), must be carefully modeled while the less important molecular diffusion term remains in a closed form. In addition, we noticed that the equally important chemistry source term $\bar{\rho} \widetilde{S_m(\Phi)}$ in Equation (51), which involves complex processes of turbulence-chemistry interaction and is very difficult to be modeled accurately, now is closed in the APDF equation with no need of modeling. This direct calculation of turbulence-chemistry interaction is one of the unique features of PDF methodology.

4.3.1 Modeling of Unclosed Terms

Consider the approximation described by Equation (54), i.e., $\bar{P} \approx \bar{\rho} R \tilde{T} / \bar{M}$, we may write from Equation (57)

$$\begin{aligned}
 -\frac{\partial \bar{P}}{\partial x_i} &\approx -\frac{\partial}{\partial x_i} \left(\frac{\bar{\rho} R \tilde{\Phi}_{M+1}}{c_v \bar{M}} \right) \\
 &= -\frac{\partial}{\partial x_i} \frac{R}{c_v \bar{M}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi_{M+1} F_{U,\Phi} d\Psi dV \\
 &= \int_{-\infty}^{\infty} V_i \frac{\partial^2}{\partial V_k \partial x_k} \left[\frac{R}{c_v \bar{M}} \int_{-\infty}^{\infty} \Psi_{M+1} F_{U,\Phi} d\Psi \right] dV \\
 &= \int_{-\infty}^{\infty} V_i \frac{\partial^2}{\partial V_k \partial x_k} \left[\frac{R}{c_v \bar{M}} \langle \Phi_{M+1} | V \rangle \cdot F_U \right] dV
 \end{aligned} \tag{66}$$

For the marginal APDF equation of F_U , we must model the unknown “conditional” mean $\langle \Phi_{M+1} | V \rangle$. While seeking its physical based model the roughest one could be suggested as follows:

$$\langle \Phi_{M+1} | V \rangle \approx \tilde{\Phi}_{M+1} = \tilde{e} \tag{67}$$

As for the term containing conditional mean, $F_\Phi \cdot \langle U_i | \Psi \rangle$, in Equation (65), we may start from a more general model for the term $\bar{\rho} \widetilde{U_i \Phi_m}$ (see Refs. 11 and 12):

$$\bar{\rho} \widetilde{U_i \Phi_m} = \bar{\rho} \tilde{U}_i \tilde{\Phi}_m - \Gamma_T^{(m)} \frac{\partial \bar{\rho} \tilde{\Phi}_m}{\partial x_i} - \Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \frac{\partial \bar{\rho} \tilde{\Phi}_m}{\partial x_j} \tag{68}$$

Where c_1, c_2 are model coefficients and were temporally set to $c_1 = c_2 = -0.24$, $\Gamma_T^{(m)}$ is the turbulent diffusivity for species Φ_m and is assumed to be the same for all species. This will lead to the following model by directly applying Equations (8) and (22) described in Sections 2.2.2 and 2.2.4:

$$F_{\Phi} \cdot \langle U_i | \Psi \rangle = \tilde{U}_i F_{\Phi} - \left[\Gamma_T^{(m)} \frac{\partial F_{\Phi}}{\partial x_i} \right] + \frac{\partial}{\partial \psi_m} \left[\Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \psi_m \frac{\partial F_{\Phi}}{\partial x_j} \right]$$

or

$$F_{\Phi} \cdot \langle U_i | \Psi \rangle = \tilde{U}_i F_{\Phi} + \frac{\partial}{\partial \psi_m} \left[\Gamma_T^{(m)} \psi_m \frac{\partial F_{\Phi}}{\partial x_i} \right] + \frac{\partial}{\partial \psi_m} \left[\Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \psi_m \frac{\partial F_{\Phi}}{\partial x_j} \right]$$

4.3.2 Summary

With the models given by Equations (66) and (69), the marginal APDF equations for $F_U(V; \mathbf{x}, t)$ and $F_{\Phi}(\Psi; \mathbf{x}, t)$ can be written as

$$\begin{aligned} \frac{\partial F_U}{\partial t} + V_j \frac{\partial F_U}{\partial x_j} = & \frac{\partial^2}{\partial V_k \partial x_k} \left[\frac{R \tilde{\Phi}_{M+1}}{c_v \bar{M}} F_U \right] + \frac{\partial}{\partial x_j} \left(\mathbf{v} \frac{\partial F_U}{\partial x_j} \right) \\ & - \frac{\partial}{\partial V_k} \left(V_j \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_k} \right) + \frac{\partial}{\partial V_k} \left(\frac{2}{3} \delta_{kj} V_m \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_m} \right) \end{aligned}$$

or

$$\begin{aligned} \frac{\partial F_U}{\partial t} + V_j \frac{\partial F_U}{\partial x_j} = & \frac{\partial^2}{\partial V_k \partial x_k} \left[\frac{R \tilde{\Phi}_{M+1}}{c_v \bar{M}} F_U \right] - \frac{\partial}{\partial V_k} \left(V_k \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_j} \right) \\ & - \frac{\partial}{\partial V_k} \left(V_j \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_k} \right) + \frac{\partial}{\partial V_k} \left(\frac{2}{3} \delta_{kj} V_m \frac{\partial}{\partial x_j} \mathbf{v} \frac{\partial F_U}{\partial x_m} \right) \end{aligned}$$

and

$$\begin{aligned} \frac{\partial F_{\Phi}}{\partial t} + \frac{\partial (\tilde{U}_i F_{\Phi})}{\partial x_i} = & \left\{ \frac{\partial}{\partial x_i} \left(\left(\Gamma^{(m)} + \Gamma_T^{(m)} \right) \frac{\partial F_{\Phi}}{\partial x_i} \right) \right\} - \frac{\partial}{\partial \psi_k} (F_{\Phi} \cdot S_k(\Psi)) \\ & - \frac{\partial}{\partial \psi_k} \left\{ \psi_k \frac{\partial}{\partial x_i} \left(\Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \frac{\partial F_{\Phi}}{\partial x_j} \right) \right\}, \quad k = 1, 2, \dots, M+1 \end{aligned}$$

or

$$\begin{aligned} \frac{\partial F_{\Phi}}{\partial t} + \frac{\partial (\tilde{U}_i F_{\Phi})}{\partial x_i} = & - \frac{\partial}{\partial \psi_k} \left\{ \psi_k \frac{\partial}{\partial x_i} \left(\left(\Gamma^{(m)} + \Gamma_T^{(m)} \right) \frac{\partial F_{\Phi}}{\partial x_i} \right) + F_{\Phi} \cdot S_k(\Psi) \right\} \\ & - \frac{\partial}{\partial \psi_k} \left\{ \psi_k \frac{\partial}{\partial x_i} \left(\Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \frac{\partial F_{\Phi}}{\partial x_j} \right) \right\}, \quad k = 1, 2, \dots, M+1 \end{aligned}$$

It can be verified that the APDF Equations (70) and (71) can exactly deduce the ensemble averaged compressible Navier-Stoke equations (48) to (51) with the assumed approximations of (66) and (68). However, the models described by Equations (66) and (69) are by no means unique. Furthermore, the variables ($\tilde{\Phi}_{M+1}$, $\tilde{U}_i$, $\tilde{S}_{ij}$ and $\tilde{\Omega}_{ij}$) are considered as available quantities during the solution procedure of APDF equations.

4.4 Conservational Form of Joint APDF $F_{U,\Phi}(V, \Psi; \mathbf{x}, t)$ Equation

The transport equation for the velocity-scalar joint APDF $F_{U,\Phi}(V, \Psi; \mathbf{x}, t)$ can be constructed from Equations (60) and (65) as

$$\begin{aligned} \frac{\partial F_{U,\Phi}}{\partial t} + V_j \frac{\partial F_{U,\Phi}}{\partial x_j} = & \frac{\partial^2}{\partial V_k \partial x_k} \left[\frac{R}{c_v \bar{M}} \int_{-\infty}^{\infty} \Psi_{M+1} F_{U,\Phi} d\Psi \right] + \frac{\partial}{\partial x_j} \left(v \frac{\partial F_{U,\Phi}}{\partial x_j} \right) \\ & - \frac{\partial}{\partial V_k} \left(V_j \frac{\partial}{\partial x_j} v \frac{\partial F_{U,\Phi}}{\partial x_k} \right) + \frac{\partial}{\partial V_k} \left(\frac{2}{3} \delta_{kj} V_\ell \frac{\partial}{\partial x_j} v \frac{\partial F_{U,\Phi}}{\partial x_\ell} \right) \\ & + \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial F_{U,\Phi}}{\partial x_i} \right) - \frac{\partial}{\partial \Psi_m} [F_{U,\Phi} \cdot S_m(\Psi)], \quad m = 1, 2, \dots, M+1 \end{aligned} \quad (72)$$

or,

$$\begin{aligned} \frac{\partial F_{U,\Phi}}{\partial t} + V_j \frac{\partial F_{U,\Phi}}{\partial x_j} = & \frac{\partial^2}{\partial V_k \partial x_k} \left[\frac{R}{c_v \bar{M}} \int_{-\infty}^{\infty} \Psi_{M+1} F_{U,\Phi} d\Psi \right] - \frac{\partial}{\partial V_k} \left(V_k \frac{\partial}{\partial x_j} v \frac{\partial F_{U,\Phi}}{\partial x_j} \right) \\ & - \frac{\partial}{\partial V_k} \left(V_j \frac{\partial}{\partial x_j} v \frac{\partial F_{U,\Phi}}{\partial x_k} \right) + \frac{\partial}{\partial V_k} \left(\frac{2}{3} \delta_{kj} V_\ell \frac{\partial}{\partial x_j} v \frac{\partial F_{U,\Phi}}{\partial x_\ell} \right) \\ & - \frac{\partial}{\partial \Psi_m} \left\{ \Psi_m \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial F_{U,\Phi}}{\partial x_i} \right) + F_{U,\Phi} \cdot S_m(\Psi) \right\}, \quad m = 1, 2, \dots, M+1 \end{aligned} \quad (73)$$

It is easy to verify that Equation (72) or (73) will reduce to Equations (70) and (71) by an integration over the entire space Ψ and V , respectively. It is noted that the transport equation for joint APDF

$F_{U,\Phi}(V, \Phi; \mathbf{x}, t)$ is in a closed form; however it contains an integration of $\int_{-\infty}^{\infty} \Psi_{M+1} F_{U,\Phi} d\Psi$ from the pressure gradient term.

5.0 Concluding Remarks

We have derived the traditional form of APDF equations by starting from the equation of FG-PDF. The resulting equations contain the “conditional means” for all the terms on the right hand side of the embedded Navier-Stokes equations except for the reaction term (see Equations (26) and (28)), which need empirical models to make the equations closed.

We have also derived the conservational form of APDF equations directly from the ensemble averaged compressible Navier-Stokes equations using the relationship between APDF and the ensemble averaged turbulent variables. In this way, the resulting joint APDF equation is in a closed form, see Equation (72) or (73).

APDF equations both in the traditional and in the conservational forms derived in this study do not subject to the low Mach number limitation.

In the marginal APDF equations, (60) and (65), there are two unclosed terms, one is related to the pressure gradient and the other is related to the scalar convection. They are generally much more important than the molecular “mixing” terms, especially at large Reynolds numbers. The models proposed in Equations (66) and (69) should be further developed and evaluated.

It should be pointed out that the methodology used in the present study can be extended to other averaging operations: for example, the Reynolds time (or spatial) averaging. Furthermore, it can also be extended to a filtering operation to derive the filtered density function (FDF) for large eddy simulation (LES) such as the mass density weighted filtered density function DW-FDF for LES of compressible turbulent reacting flows (see Ref. 6).

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